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LES, DNS and RANS for the Analysis of High-Speed Turbulent Reacting Flows

by

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Abstract

The purpose of this research is to continue our efforts in advancing the state of knowledge in large eddy simulation (LES), direct numerical simulation (DNS) and Reynolds averaged Navier Stokes (RANS) methods for the computational analysis of high-speed reacting turbulent flows. We are currently in the third year of Phase II of this research. This semi-annual report provides a brief and up-to-date summary of our activities during the past six months covering the period: August 1, 1995 through January 31, 1996.

Technical Monitor:

Dr. J. Philip Drummond (Hypersonic Propulsion Branch, NASA LaRC, Mail Stop 197, Tel: 804-864-2298) is the Technical Monitor of this Grant.

Summary of Achievements

We are now in Year 3 of the Phase II activities on this NASA LaRC sponsored project. The total time allotted for this phase is three years; this phase was followed at the conclusion of Phase I activities (also for three years). Thus, in total we have completed $5\frac{1}{2}$ years of LaRC supported research, and one half year is remaining.

The scope of our activities are determined and continuously appraised and modified via interactions with NASA LaRC. Based on our to-date achievements and the recommendations made by NASA LaRC, our efforts are presently concentrated on four major tasks: **(1)** Development and implementation of an efficient Monte Carlo computational procedure for LES of chemically reactive turbulent flows. **(2)** Development of algebraic moment closures for statistical description of compressible flows. **(3)** Implementation of the algebraic closures as developed in (2) in the computer code LARCK. **(4)** Application of the LES code as developed in (1) for simulations of flows of interest to NASA LaRC. Below. a summary is provided of our accomplishments in each of the four constituents of our activities.

Task 1:

Our efforts in task (1) have been particularly fruitful within the past six months. We have managed to formulate the probability density function (PDF) of scalars within the subgrid and to develop a very efficient Monte Carlo numerical procedure for the solution of this PDF in LES of chemically reactive flows. As we indicated in our last report, it appears impossible to implement the subgrid PDF in the conventional Eulerian context; Lagrangian procedure appears to be the *only* means of treating this PDF numerically. There are, however, several "subtle" issues which need to (and are being) resolved. The essential element of the Lagrangian descriptor is to treat the PDF via an ensemble of computational "particles" representing the PDF. The transport and (more importantly) the "dispersion" of these particles can be only described by "Stochastic Differential Equations" (SDEs). These SDEs are constructed in such a way to, hopefully, portray the essential physics. Numerical implementation of Lagrangian Monte Carlo methods have yielded promising results. Two-dimensional nonpremixed reacting mixing layers and jet configurations have been considered to assess the performance of both the models and the numerical techniques. Because of the particular representation offered by the Lagrangian technique, special problems involving mean transport must be overcome that are not relevant in the case of RANS. At the moment, this area is in the developmental phase.

It must be mentioned that in all our efforts in this task, we have only considered the (joint) PDF of "scalar" quantities. We have not extended the methodology for consideration of the joint PDF of velocity and scalars. Based on our preliminary assessments, this extension requires long-term planning and we must seek the permission of NASA LaRC before committing to this task.

It must also be mentioned that we are collaborating with Professor Stephen B. Pope of Cornell University in resolving several theoretical issues pertaining to this task.

Task 2:

Our efforts in this task within the past six months have been primarily concentrated on two sub-tasks : (i) Development of algebraic moment closures for statistical description of highly compressible flows described in a general coordinate system, and (ii) implementation and assessment of the models for free shear flows for which experimental data are available. Recently, several important aspects have been recognized about the nature of the turbulent state of a compressible medium and progress has been made in advancing the modeling of simple flows, but the inclusion of compressibility effects and of variable inertia effects in the models is still a difficult undertaking, especially for the second-order moment closures. Previous contributions have exploited the decomposition concept of the compressible field to generate models for terms specific to high-speed flows, *i.e.* the pressure dilatation and the dilatational dissipation. These terms have been perceived to contribute to the reduced growth rate of the compressible mixing layer. These models have been applied in many instances as compressibility corrections in conjunction with the $k-\epsilon$ model or with the actualize incompressible Reynolds stress turbulence model. By contrast true compressible second-order models are scarcely available. In an attempt to overcome this deficiency, in this work linear closures for the pressure-strain and the pressure-scalar gradient correlations are proposed and simple models for the averaged Favré scalar fluctuations are derived. Based on the above models, we have succeeded in providing explicit algebraic relations for the Reynolds stresses and for the "turbulent flux" of scalar variables in high-speed flows. These models have been extended for a non-orthogonal curvilinear coordinate system. Both non-reacting and reacting flows with heat release are considered. In the latter, a second-order irreversible chemical reaction in considered in turbulent flows with initially segregated reactants. The closures explicitly account for the influence of the turbulent Mach number, the Damköhler number, the density gradient, the pressure gradient and the mean dilatation effects. The methodology is being applied for prediction of non-premixed, heat-releasing spatially developing turbulent free shear-layers (including mixing layers and planar jets) over a wide range of Mach numbers. The numerical solution procedure for the integration of the governing equations is based on several predictor-corrector finite difference schemes: McCormack, Gottlieb-Turkel and Carpenter with a local time stepping technique, to accelerate the convergence towards the steady-state solution. The implementation of the models is completed and we are in the testing phase. The assessment of the closures is performed in relation to currently available experimental data for highly compressible free-shear flows.

Our efforts within the next six months will be mostly concentrated on numerical simulations of compressible turbulent shear flows and verifications of the results via comparison with laboratory data.

<u>**Task 3:**</u>

In our efforts pertaining to (3), we have been successful in implementing our algebraic turbulent Reynolds stress models in the computer code LARCK (Langley Algorithm for Research in Chemical Kinetics) developed at the NASA Langley Research Center. In the computational procedure, the multi-grid procedure is used along with an elliptic solver in order to accelerate convergence to steady state. Within the past 6 months, we have implemented the incompressible version of the algebraic Reynolds stress model into the code and have verified the results via those previously obtained with this model but with a different code. We are now in the process of implementing the algebraic scalar flux model, still in incompressible flow, into the code.

We have not started the implementation of the compressible algebraic model (as developed in (2)) into the LARCK code yet. We must seek the permission of NASA LaRC before committing to this task.

<u>**Task 4:**</u>

Finally, in our efforts pertaining to (4), we have started work on LES of flows of interest to NASA LaRC. For this task, we have completed the modification of our LES-PDF code to three-dimension making it suitable for the simulations of practical flows. However, we do not have any results to report, because the graduate student working on this project has been preparing for the Ph.D. qualifier examination within the past 4-5 months. This exam will be concluded in mid February 1996. Therefore, within the next 6 months we will hopefully have some time to devote to this task. The extent of our efforts on this task will depend on current & future priorities and goals at the NASA LaRC.

Personnel

The Co-PIs of this project are Drs. Peyman Givi and Dale B. Taulbee. Two Graduate Research Assistants (RAs) are being supported directly by this Grant: (1) Mr. Paul Colucci and (2) Mr. Virgil Adumitroaie. Mr. Colucci is involved in task (1) and Mr. Adumitroaie is responsible for task (2).

However, considering the diversity of this research we have had to involve several additional students. The following students are also contributing to this project but are not financially supported by NASA: Mr. Farhad Jaberi, Mr. Laurent Gicquel and Mr. Sean Garrick. Mr. Jaberi is assisting Mr. Colucci in task (1), Mr. Gicquel is solely responsible for task (3) and Mr. Garrick is responsible for task (4).